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Unified kriging metamodel for deterministic and noise information

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ABSTRACT

Kriging model is widely used as a design analysis and computer experiment (DACE) model in the field of engineering design to accomplish computationally feasible design optimization. In general, kriging model has been applied to many engineering applications as an interpolation model because it is usually obtained based on deterministic computer experiemnts [1]. But if the response includes not only global nonlinearity but also noise like numerical errors, it is inappropriate to use conventional kriging model that can distort global characterisitic. In this research, unified kriging model that can represent both interpolation and smoothing is proposed. The performances of unified kriging model are compared with those of interpolating kriging model for analytical function with error of trigonometric function type.

Unified kriging model postulates the random response as the combination of a polynomial model, departure from the polynomial model and random errors, i.e.,

$$Y(\mathbf{x}) = \mathbf{f}(\mathbf{x})^T \boldsymbol{\beta} + z(\mathbf{x}) + \varepsilon_r(\mathbf{x}) \tag{1}$$

where $\mathbf{f}(\mathbf{x}) = \{f_1(\mathbf{x}), f_2(\mathbf{x}), \cdots, f_p(\mathbf{x})\}^T$ is known function vector that is defined as variables $\mathbf{x} \in R^{n_d}$ and $\boldsymbol{\beta} = \{b_1, b_2, \cdots, b_p\}^T$ is unknown regression coefficient vector, respectively. Note that deviation $z(\mathbf{x})$ and random error $\varepsilon_r(\mathbf{x})$ follow independently $N(0, \sigma_z^2 \mathbf{V})$ and $N(0, \sigma_\varepsilon^2)$, respectively. Because the deviation and random error are independent, the correlation between any two responses $Y(\mathbf{x}^i)$ and $Y(\mathbf{x}^j)$ can be represented as follows:

$$\begin{aligned} \mathrm{cov}[Y(\mathbf{x}^i), Y(\mathbf{x}^j)] &= \mathrm{cov}[z(\mathbf{x}^i), z(\mathbf{x}^j)] + \mathrm{cov}[\varepsilon_r(\mathbf{x}^i), \varepsilon_r(\mathbf{x}^j)] \\ &= \sigma_z^2 \left[\exp\left(-\sum_{k=1}^{n_d} \theta_k (x_k^i - x_k^j)^{\alpha_k} \right) + \gamma \right] \equiv \sigma_z^2 \mathbf{V} \end{aligned} \tag{2}$$

where $\gamma = \sigma_\varepsilon^2 / \sigma_z^2$ denotes the variance ratio of random error with respect to the response.

The unified kriging is now derived by means of finding the best linear unbiased predictor (BLUP) that minimizes the mean squared error among all linear predictors while satisfying unbiasedness as follows [2, 3]:

$$\hat{Y}(\mathbf{x}) = \mathbf{f}(\mathbf{x})^T \hat{\boldsymbol{\beta}} + \mathbf{v}(\mathbf{x})^T \mathbf{V}^{-1} (\mathbf{Y} - \mathbf{F}\hat{\boldsymbol{\beta}}) \tag{3}$$

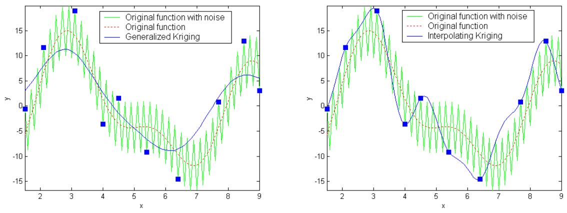
where $\hat{\boldsymbol{\beta}} = (\mathbf{F}^T \mathbf{V}^{-1} \mathbf{F})^{-1} \mathbf{F}^T \mathbf{V}^{-1} \mathbf{Y}$ is generalized least square estimator. The unknown parameters $\theta_k, \alpha_k, \gamma$ are determined by maximum likelihood estimation as follows:

$$\underset{\boldsymbol{\theta}, \boldsymbol{\alpha}, \gamma}{\text{minimize}} \;\; \hat{\sigma}_z^2 |\mathbf{V}|^{1/n} \;\; \text{subject to } \theta_k > 0;\; 0 < \alpha_k \le 2;\; 0 \le \gamma \le 1;\; k = 1, 2, \cdots, n_d \tag{4}$$

Let us consider a test function with error of trigonometric type that has high frequency as follows:

$$y(x) = 10\sin(\frac{\pi}{3} + 10)\sin(\frac{\pi}{3}x) - 10\cos(\frac{\pi}{3}x) + 5\sin(\frac{\pi}{8}x) + \varepsilon_r;\; x \in [1,\ 9],\;\; \varepsilon_r = 5\cos(10\pi x) \tag{5}$$

Fig. 1 (a) denotes the unified kriging model and conventional kriging model with 10 sample points. The accuracy of the interpolating kriging model is inaccurate in the prediction of inflection points and global minimum. However, unified kriging model shows excellent of the prediction for global feature of response as well as the location of global maximum. In the contrast with unified kriging model, the interpolating kriging model has several local minima, which means that interpolation strategy has a negative influence on approximation for responses with random errors.



(a) (b)

Fig. 1 Metamodels: (a) unified kriging model and (b) interpolating kriging model

Table 1 summarizes the results of MLE for both kriging models. Variance ratio of random error with respect to response $\hat{g}$ is given in Table 1. From a statistical meaning, the value of likelihood function indicates that unified kriging model is more suitable than interpolating kriging model.

Unified kriging model that both interpolates and smoothing in according to the type of response is proposed. Maximum likelihood estimation of unified kriging model is compared with that of interpolating kriging model for a function with numerical noise. As a result, for unified kriging model, the smaller q_k and the larger g_k, the more smooth is curvature of unified kriging model. For the test example, we can find that unified kriging model has not only robustness for numerical noise but also can express the global behavior of response effectively.

Table 1 Parameters from MLE process

Estimation	Unified Kriging	Interpolating Kriging
$\hat{b}$	–0.126	–0.073
$\hat{s}_z^2$	99.751	102.012
$\hat{q}_1$	5.485	18.434
$\hat{a}_1$	2.00	2.000
$\hat{g}$	0.418	0.000
MLE	0.841	0.893

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